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(54) Title: PHARMACOKINETIC–BASED DRUG DESIGN TOOL AND METHOD

(57) Abstract

The present invention relates to a pharmacokinetic–based design and selection tool (PK tool) and methods for predicting absoption of an administered compound of interest. The methods utilize the tools, and optionally a separately operable component or subsystem thereof. The PK tool includes as computer–readable components: (1) input/output system; (2) physiologic–based simulation model of one or more segments of a mammalian system of interest having one or more physiological barriers to absorption that is based on the selected route of administration; and (3) simulation engine having a differential equation solver. The invention also provides methods for optimizing as well as enabling minimal input requirements a physiologic–based simulation model for predicting *in vivo* absorption, and optionally one or more additional properties, from either *in vitro* or *in vivo* data. The PK tool of the invention may be provided as a computer system, as an article of manufacture in the form of a computer–readable medium, or a computer program product and the like. Subsystems and individual components of the PK tool also can be utilized and adapted in a variety of disparate applications for predicting the fate of an administered compound. The PK tool and methods of the invention can be used to screen and design compound libraries, select and design drugs, as well as predict drug efficacy in mammals from *in vitro* and/or *in vivo* data of one or more compounds of interest. The PK tool and methods of the invention also find use in selecting, designing, and preparing drug compounds, and multi–compound drugs and drug formulations (i.e., drug delivery system) for preparation of medicaments for use in treating mammalian disorders.